## Model Performance

| Model | Data |
|---|---|

### Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|---|---|---|---|---|---|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.85 | 1.14 | 0.85 | 1.12 | 0.83 | 1.23 |

## Model Results

**Predicted value:** 3.18e-11 cm3/molecule*sec

**Global applicability domain:** Outside

**Local applicability domain index:** 2.59e-01

**Confidence level:** 7.10e-01

## Nearest Neighbors from the Training Set

Image not found
1,3,5-Cycloheptatriene
**Measured:** 9.69e-11
**Predicted:** 1.00e-10

Image not found
1,4-Benzoquinone
**Measured:** 4.60e-12
**Predicted:** 5.97e-12

Image not found
(2E)-3-Phenylprop-2-enal
**Measured:** 4.80e-11
**Predicted:** 5.31e-11

Image not found
2-Methyl-p-benzoquinone
**Measured:** 2.35e-11
**Predicted:** 2.15e-11